Category	Chemicals from Blanket Wash Use Cluster in Category
Hydrocarbons, aromatic	Benzene, 1, 2, 4-trimethyl-; Cumene; Solvent naphtha (petroleum), heavy aromatic; Solvent naphtha (petroleum), light aromatic; Xylene
Hydrocarbons, petroleum distillates	Distillates (petroleum), hydrotreated middle; Mineral spirits (light hydrotreated); Naphtha (petroleum), hydrotreated heavy; Solvent naphtha (petroleum), light aliphatic (VM&P Naphtha); Solvent naphtha (petroleum), medium aliphatic; Stoddard solvent
Esters/lactones	Butyrolactone; Propanoic acid, 3-ethoxy-, ethyl ester; Sodium bis(ethylhexyl) sulfosuccinate; Sorbitan tri-9-octadecenoate, poly(oxy-1,2-ethanediyl) derivatives
Nitrogen heterocyclics	N-methyl pyrrolidone
Propylene glycol ethers	Dipropylene glycol monobutyl ether; Dipropylene glycol methyl ether; Propylene glycol monobutyl ether;
Terpenes	Hydrocarbons, terpene processing by-products; <i>d</i> -Limonene; Linalool; Nerol; 2-Pinanol; Plinols; α-Terpineol; Terpinolene;

2.2 CHEMICAL INFORMATION

This section discusses the physical nature of the 56 specific chemicals used in blanket wash formulations. First, there is a description of the types of information that are provided for each chemical, including a glossary of chemical properties terms presented in Table 2-2. This includes their chemical and physical properties, safety hazard factors, and environmental fate. Following these descriptions, Table 2-3 lists the name, Chemical Abstracts Service (CAS) Registry Number, and common synonyms for each of the chemicals. The chemical and physical properties and safety hazard factors are then listed in the Chemical Properties and Information summary for each chemical.

2.2.1 Chemical Properties and Information

For each blanket wash chemical, there is a corresponding Chemical Properties and Information summary. All of the information in these summaries, except for the Safety Hazard Factors, was obtained by searching standard references, listed at the end of this chapter. This summary contains information on the following chemical and physical properties:

Table 2-2. Glossary of Chemical Properties Terms

_	- n	
<u>Term</u>	<u>Definition</u>	
Chemical Abstracts Service Registry Number (CAS #)	A unique identification code, up to ten digits long, assigned to each chemical registered by the Chemical Abstract Service. The CAS # is useful when searching for information on a chemical with more than one name.	
Synonyms	Alternative names commonly used for the chemical.	
Molecular weight	A summation of the individual atomic weights based on the numbers and kinds of atoms present in a molecule of a chemical substance. For polymers, this may include molecular weight distributions, ranges, and averages. Typical unit is g/mole.	
Melting point	The temperature at which a substance changes from the solid to the liquid state. It indicates at what temperature solid substances liquify. Typical unit is °C.	
Water solubility	The maximum amount of a chemical that can be dissolved in a given amount of pure water at standard conditions of temperature and pressure. Typical unit is g/L.	
Vapor pressure	The pressure exerted by a chemical in the vapor phase in equilibrium with its solid or liquid forms. It provides an indication of the relative tendency of a substance to volatilize. Typical unit is mm Hg.	
Octanol-water partition coefficient (Log ₁₀ K _{ow})	Provides a measure of the extent of a chemical partitioning between water and octanol (as a surrogate for lipids or other organics) at equilibrium. It is an important parameter because it provides an indication of a chemical's water solubility and its propensity to bioconcentrate in aquatic organisms or sorb to soil and sediment.	
Soil sorption coefficient (Log ₁₀ K _{oc})	Provides a measure of the extent of chemical partitioning between the solid and solution phases of a two-phase system, especially soil, sediment or activated sludge. Usually expressed on an organic carbon basis, as the equilibrium ratio of the amount of chemical sorbed per unit weight of organic carbon in the soil, sediment or sludge to the concentration of the chemical in solution. The higher the $K_{\rm oc}$, the more likely a chemical is to bind to soil or sediment than to remain in water.	
Bioconcentration factor (Log ₁₀ BCF)	Provides a measure of the extent of chemical partitioning at equilibrium between a biological medium such as fish tissue or plant tissue and an external medium such as water. The higher the BCF, the greater the accumulation in living tissue is likely to be.	
Henry's Law Constant	Provides a measure of the extent of chemical partitioning between air and water at equilibrium; estimated by dividing the vapor pressure of a sparingly water soluble chemical substance by its water solubility. The higher the Henry's Law constant, the more likely a chemical is to volatilize than to remain in water.	
Publicly Owned Treatment Works (POTW) overall removal rate	The extent to which a chemical substance is removed from influent wastewater by typical POTWs employing activated sludge secondary treatment. Expressed as 100 minus that percentage of the material originally present that remains in the liquid effluent after treatment.	
Chemistry of use	The primary use of the chemical in the lithographic printing industry.	

Molecular formula and physical structure of the chemical	A description of the number and type of each atom in the chemical and a description of how the atoms are arranged and the types of bonds between atoms.
Boiling point	The temperature at which a liquid under standard atmospheric pressure (or other specified pressure) changes from a liquid to a gaseous state. It is an indication of the volatility of a substance. The distillation range in a separation process, the temperature at which the more volatile liquid of a mixture forms a vapor, is used for mixtures in the absence of a boiling point. Typical unit is °C.
Density	The mass of a liquid, solid, or gas per unit volume of that substance, i.e., the mass in grams contained in 1 cubic centimeter of a substance at 20°C and 1 atmosphere pressure. Typical unit is g/cm ³ .
Flash point	The minimum temperature at which a liquid gives off sufficient vapor to form an ignitible mixture with air near the surface of the liquid or within the test vessel used.
Safety hazard factors	Discussed in detail below.

Any of the property values acquired from the standard references have been designated as measured (M), since the data in these sources have been experimentally determined for the specific chemical in question. (Please note that synonyms, molecular weight, chemistry of use, and structure have no such designation since these are not values that can be measured, but rather are attributes intrinsic to the chemical in question.)

For some chemicals there was little or no information in the standard references and significant data gaps existed. Therefore, the values for the physical and chemical properties of these chemicals needed to be estimated. These estimations were obtained using several programs accessed through the Estimation Programs Interface (EPI), available from Syracuse Research Corporation. EPI uses the structure of the chemical for input to eight chemical property estimation programs. The programs used to complete the individual Chemical Properties and Information summaries are as follows:

- Octanol-Water Partition Coefficient Program (LOGKOW). (Meylan WM and PH Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84: 83-92.)
- Henry's Law Constant Program (HENRY). (Meylan WM and PH Howard. 1991.
 Bond contribution method for estimating Henry's Law constants. Environ. Toxicol.
 Chem. 10:1283-1293.)
- Soil Sorption Coefficient Program (PCKOC). (Meylan WM, PH Howard and RS Boethling. 1992. Molecular topology/fragment contribution method for predicting soil sorption coefficients. Environ. Sci. Technol. 26:1560-1567.)
- Melting Point, Boiling Point, Vapor Pressure Estimation Program (MPBPVP).
- Water Solubility Estimation Program (WSKOW). (Meylan WM, PH Howard and RS Boethling. 1996. Improved method for estimating water solubility from octanol/water coefficient. Environ Toxicol. Chem. 15(2):100-106.)

• Sewage Treatment Plant Model (STP), a fugacity model for estimating the efficiency of pollutant removal. (Clark B, JG Henry and D Mackay. 1995. Fugacity analysis and model of organic chemical fate in a sewage treatment plant. Environ. Sci. Technol. 29:1488-1494.)

The accuracy of these programs has not been established in all cases, but the listed programs are considered to be the best methods currently available. In addition to the journal articles discussing the development and use of these programs found at the end of this section (with the exception of the MPBPVP program), a user's guide also is available for the EPI and each program. Any property values determined using these programs have been designated as estimated (E). It should be noted that the water solubility estimation program has an anticipated margin of error of plus or minus one order of magnitude. The LOGKOW is expected to be accurate to 0.1 log units for most compounds, although the PCKOC is likely to be somewhat less accurate due to the complex nature of the soil/sediment sorption phenomena.

For several chemicals, no data were available in any of the primary sources, and EPI estimation methods were not performed because the complex nature of the chemical (e.g., chemicals with ranges of carbon atoms) skewed the estimation results. For these chemicals, chemical and physical data had to be estimated based on structure-activity relationships (i.e., comparison with analogous chemicals with known properties). In addition, some properties were estimated from best chemical judgment based on the class of compounds to which the chemical in question belongs. For example, chemical and physical property values for benzenesulfonic acid, dodecyl-, compounds with 2-aminoethanol have been estimated based on similarities with the other benzenesulfonic dodecyl- blanket wash chemicals. Any property values determined by this comparison method have been designated by an (E), estimated. Any chemical and physical property values that still could not be estimated have been designated as not available.

2.2.2 Safety Hazard Factors

In addition to the physical and chemical properties of a chemical discussed above, there are other chemical attributes that are important for the handling, use and storage of a chemical in the workplace. These attributes have been designated as Safety Hazard Factors and they include chemical reactivity, flammability, ignitability and corrosivity. Information used to determine the Safety Hazard Factors was taken from the following sources (if information was not available for particular factor it was not included in the Chemical Properties and Information summary):

- National Fire Protection Association's (NFPA) Fire Protection Guide to Hazardous Materials (10th edition), Quincy, Massachusetts.
- 40 CFR §261.20 (Protection of Environment, RCRA, Identification and Listing of Hazardous Waste), Characteristic of Ignitability.
- Department of Transportation's Hazardous Materials Table 49 CFR §172.101.

The reactivity and flammability values are taken from the National Fire Protection Association's (NFPA) Fire Protection Guide to Hazardous Materials (10th edition). For reactivity, materials are ranked on a scale of 0 through 4:

- 0 materials that are normally stable, even under fire exposure conditions, and that do not react with water; normal fire fighting procedures may be used.
- 1 materials that are normally stable, but may become unstable at elevated temperatures and pressures and materials that will react with water with some

- release of energy, but not violently; fires involving these materials should be approached with caution.
- 2 materials that are normally unstable and readily undergo violent chemical change, but are not capable of detonation; this includes materials that can rapidly release energy, materials that can undergo violent chemical changes at high temperatures and pressures, and materials that react violently with water. In advanced or massive fires involving these materials, fire fighting should be done from a safe distance of from a protected location.
- 3 materials that, in themselves, are capable of detonation, explosive decomposition, or explosive reaction, but require a strong initiating source or heating under confinement; fires involving these materials should be fought from a protected location.
- 4 materials that, in themselves, are readily capable of detonation, explosive decomposition, or explosive reaction at normal temperatures and pressures. If a material having this Reactivity Hazard Rating is involved in a fire, the area should be immediately evacuated.

For flammability, materials are ranked on a scale of 0 through 4:

- 0 any material that will not burn.
- 1 materials that must be preheated before ignition will occur and whose flash point exceeds 200°F (93.4°C), as well as most ordinary combustible materials.
- 2 materials that must be moderately heated before ignition will occur and that readily give off ignitible vapors.
- 3 flammable liquids and materials that can be easily ignited under almost all normal temperature conditions. Water may be ineffective in controlling or extinguishing fires in such materials.
- 4 includes flammable gases, pyrophoric liquids, and flammable liquids. The preferred method of fire attack is to stop the flow of material or to protect exposures while allowing the fire to burn itself out.

Chemicals not ranked by NFPA were not assigned a reactivity or a flammability value.

For ignitability, the blanket wash chemicals have been classified as either ignitable "Y", or not ignitable "N". The determination of ignitability is based upon the standard outlined in 40 CFR §261.20 (Protection of Environment, RCRA; Identification and Listing of Hazardous Waste), Characteristic of Ignitability. Under this standard, a chemical is considered ignitable if it "is a liquid, other than an aqueous solution containing less than 24 percent alcohol by volume and has a flash point less than 60°C (140°F) as determined by a Pensky-Martens Closed Cup Tester...a Setaflash Closed Cup Tester...or an equivalent test method." The flash points for these chemicals were taken from the NFPA Fire Protection Guide to Hazardous Materials, and if no flash point existed for a chemical, no ignitability designation was assigned.

For corrosivity, the blanket wash chemicals have been categorized as either corrosive or not corrosive. Any chemical with a designation in the corrosivity column is listed in the Department of Transportation's Hazardous Materials Table in 49 CFR §172.101. This table lists all required labels a chemical must have affixed to its container prior to shipping. Chemicals

which require a corrosive shipping label have been designated by "Y", while chemicals which do not require this label have been designated by "N". Chemicals not listed in the DOT Hazardous Materials Table have not been assigned a corrosivity designation.

2.2.3 Chemical Properties and Information Summaries

In Table 2-3, each of the 56 blanket wash chemicals are listed along with their common synonyms and the Chemical Abstracts Service Registry Number. Immediately following the table are the individual Chemical Properties and Information summaries for each chemical.

Table 2-3. Chemicals in Blanket Wash Formulations

Chemical Name	CAS Number	Synonym
Alcohols, C ₁₂ -C ₁₅ , ethoxylated ^c	68131-39-5	EMUL/Mix ^b
Benzene, 1,2,4-trimethyl-	95-63-6	Pseudocumene
Benzenesulfonic acid, dodecyl-°	27176-87-0	Dodecyl benzene sulfonic acid ^b
Benzenesulfonic acid, dodecyl-, compounds with 2-aminoethanol	26836-07-7	Dodecylbenzenesulfonic acid, ethanolamine salt
Benzenesulfonic acid, dodecyl-, compounds with 2-propanamine ^c	26264-05-1	Isopropylamine salt of dodecylbenzenesulfonic acid ^b
Benzenesulfonic acid, (tetrapropenyl)-, compounds with 2- propanamine	157966-96-6	Isopropylamine salt of (tetrapropenyl) benzenesulfonic acid
Benzenesulfonic acid, C ₁₀ -C ₁₆ - alkyl derivatives, compounds with 2-propanamine ^c	68584-24-7	Benzenesulfonic acid, C ₁₀ -C ₁₆ - alkyl derivatives, compounds with isopropylamine
Butyrolactone	96-48-0	2(3H)-Furanone, dihydro ^b
Cumene ^a	98-82-8	Benzene, (1-methylethyl)-b
Diethanolamine ^a	111-42-2	Ethanol, 2,2'-iminobis-b
Diethylene glycol monobutyl ether	112-34-5	Ethanol, 2-(2-butoxyethoxy)-b
Dimethyl adipate	627-93-0	Dimethyl hexanedioate; methyl adipate; dimethyl ester adipic acid
Dimethyl glutarate	1119-40-0	Glutaric acid, dimethyl ester; pentanedioic acid, dimethyl ester
Dimethyl succinate	106-65-0	Succinic acid, dimethyl ester; butanedioic acid, dimethyl ester; methyl succinate
Dipropylene glycol monobutyl ether	29911-28-2	2-Propanol, 1-(2-butoxy-1- methylethoxy)- ^b DGMBE
Dipropylene glycol methyl ether	34590-94-8	DPGME
Distillates (petroleum), hydrotreated middle ^c	64742-46-7	Hydrotreated middle distillate ^b

Chemical Name	CAS Number	Synonym
Ethoxylated nonylphenol	9016-45-9 26027-38-3 68412-54-4	Ethoxylated nonylphenol ^b , α-(nonylphenyl)-ω-hydroxy-, branched and unbranched isomers ^c ; NP-6 ^b ; NP-9 ^b
Ethylenediaminetetraacetic acid, tetrasodium salt	64-02-8	Tetrasodium EDTA
Fatty acids, C ₁₆ -C ₁₈ , methyl esters ^c	67762-38-3	Fatty acid methyl esters ^b
Fatty acids, C ₁₆ -C ₁₈ and C ₁₈ -unsatd, compounds with diethanolamine ^a	68002-82-4	Diethanolamine tallate ^b
Fatty acids, tall oil, compounds with diethanolamine	61790-69-0	Diethanolamine tallate
Hydrocarbons, terpene processing by-products ^c	68956-56-9	
<i>d</i> -Limonene ^a	5989-27-5	Cyclohexene, 1-methyl-4-(1-methylethenyl)- ^b ; Terpenes ^b
Linalool ^a	78-70-6	1,6-Octadien-3-ol, 3,7-dimethyl- ^b
Mineral spirits (light hydrotreated)	64742-47-8	Petroleum distillate ^b
N-Methylpyrrolidone	872-50-4	NMP
Naphtha (petroleum), hydrotreated heavy ^c	64742-48-9	Aliphatic petroleum distillate C ₉ -C ₁₁ ^b
Nerol ^a	106-25-2	2,6-Octadien-1-ol, 3,7-dimethyl-b
Oxirane, methyl, polymer with oxirane, monodecyl ether ^c	37251-67-5	Linear alkyl ethoxylate ^b
2-Pinanol ^a	473-54-1	Bicyclo[3.1.1]heptan-2-ol, 2,6,6- trimethyl- ^b
Plinols ^b	72402-00-7	Cyclopentanol, 1,2-dimethyl-3-(1-methylethenyl)-°
Polyethoxylated isodecyloxypropylamine ^b	68478-95-5	Poly(oxy-1,2-ethanediyl), α,α'-(iminodi- 2,1-ethanediyl)bis[ω-hydroxy]-, N-[3- (branched decyloxy)propyl] derivatives°
Poly(oxy-1,2-ethanediyl), α-hexyl-ω- hydroxy-°	31726-34-8	Ethoxylated hexyl alcohol
Propanoic acid, 3-ethoxy-, ethyl ester ^a	763-69-9	Ethyl-3-ethoxy propionate
Propylene glycol	57-55-6	1,2-Propanediol
Propylene glycol monobutyl ether	5131-66-8	2-Propanol, 1-butoxy- ^b
Sodium bis(ethylhexyl) sulfosuccinate ^b	577-11-7	Butanedioic acid, sulfo-, 1,4-bis(2- ethylhexyl) ester, sodium salt ^c
Sodium hydroxide	1310-73-2	Caustic soda

Chemical Name	CAS Number	Synonym
Sodium xylene sulfonate ^b	1300-72-7	Benzenesulfonic acid, dimethyl-, sodium salt°
Solvent naphtha (petroleum), heavy aromatic	64742-94-5	Aromatic 150 ^b
Solvent naphtha (petroleum), light aliphatic	64742-89-8	VM&P naphtha ^b
Solvent naphtha (petroleum), light aromatic	64742-95-6	Aromatic petroleum distillate C ₈ -C ₁₁ ^b
Solvent naphtha (petroleum), medium aliphatic°	64742-88-7	Solvent 140 ^b
Sorbitan, mono-9-octadecenoate ^c	1338-43-8	Sorbitan mono-oleate (crillet 4) ^b
Sorbitan, monododecanoate, poly(oxy-1,2-ethanediyl) derivatives ^c	9005-64-5	Laurate of polyoxyethylenic sorbitan ^b
Sorbitan, monolaurate	5959-89-7	D-Glucitol, 1,4-anhydro-, 6- dodecanoate ^b
Sorbitan, tri-9-octadecenoate, poly(oxy-1,2-ethanediyl) derivatives°	9005-70-3	Ethoxylated sorbitan tri-oleate (crillet 45) ^b
Soybean oil, methyl ester ^c	67784-80-9	Soybean based methyl esters ^b
Soybean oil, polymerized, oxidized ^c	68152-81-8	Oxidized soybean oil ^b
Stoddard solvent ^a	8052-41-3	Mineral spirits
Tall oil, special	68937-81-5	Special tall oil ^b methyl stearate, methyl oleate
α-Terpineol ^a	98-55-5	3-Cyclohexene-1-methanol, α , α , 4-trimethyl- $^{\text{b}}$
Terpinolene ^a	586-62-9	Cyclohexene, 1-methyl-4-(1-methylethylidene)- ^b
Tetrapotassium pyrophosphate ^b	7320-34-5	Diphosphoric acid, tetrapotassium salta
Xylene	1330-20-7	Dimethyl benzene

a Indicates that the name was chosen from the CHEMID Files.
b Indicates name supplied by industry.
c Indicates that the name was chosen from the TSCA Inventory.

Alcohols, C₁₂-C₁₅, Ethoxylated

CAS# 68131-39-5

Chemical Properties and Information

Synonyms: ethoxylated fatty alcohols; EMUL/Mix

Molecular weight: >200 Melting Point: <50°C (E)

Water Solubility: Dispersable (n=3 to 10) (E)

Vapor Pressure: <0.01 mm Hg (E)

 $Log_{10}K_{ow}$: 3.40 (E) $Log_{10}K_{oc}$: 3.97 (E) $Log_{10}BCF$: 2.35 (E)

Henry's Law: <1.00X10⁻⁸ atm-m³/mol (E) POTW Overall Removal Rate (%): 83-99 (E)

Chemistry of Use: Dispersant

Molecular formula varies

Structure:

 $R(OCH_2CH_2)_nOH$

 $R = C_{12} \text{ to } C_{15}$

Boiling Point: Decomposes (E)

Density: 0.95 g/cm³ (E)
Flash Point: >100°C (E)
Safety Hazard Factors:

Ignitability: N

Above data are either measured (M) or estimated (E)

Benzene, 1,2,4-Trimethyl

CAS# 95-63-6

Chemical Properties and Information

Synonyms: 1,2,4-trimethyl benzene;

pseudocumene;

trimethyl benzene; asymmetrical trimethyl

benzene

Molecular weight: 120.19 Melting Point: -43.78°C (M) Water Solubility: 0.02 g/L (E)

Vapor Pressure: 10.34 torr (at 54.4°C) (M)

Log₁₀K_{ow}: 3.78 (M) Log₁₀K_{oc}: 2.86 (M) Log₁₀BCF: 2.53 (E)

Henry's Law: 6.58X10⁻³ atm-m³/mole (M) POTW Overall Removal Rate (%): 97-99 (E) Chemistry of Use: Solvent component C₉H₁₂ Structure:

 CH_3

Boiling Point: 169 -171°C (M) Density: 0.876 g/cm³ (M) Flash Point: 54.4°C (M) Safety Hazard Factors:

Reactivity: 0 Flammability: 2 Ignitability: N

Benzenesulfonic Acid, Dodecyl-

CAS# 27176-87-0

Chemical Properties and Information

Synonyms: DDBSA
Molecular weight: 326
Melting Point: Not available
Water Solubility: Miscible (E)
Vapor Pressure: <10⁻⁴ mm Hg (E)

Log₁₀K_{ow}: 4.78 (E) Log₁₀K_{oc}: 4.23 (E) Log₁₀BCF: 3.41 (E)

Henry's Law: 6.27X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 99.82-99.98

(E)

Chemistry of Use: Surfactant

C₁₈H₃₀SO₃ Structure:

C₁₂H₂₅ SOH

Boiling Point: 204.5°C (M) Density: 1.00 g/cm³ (M)

Flash Point: 149° C (open cup) (M)

Safety Hazard Factors:

Corrosivity: Y

Above data are either measured (M) or estimated (E)

Benzenesulfonic Acid, Dodecyl-, Compounds with 2-Aminoethanol

CAS# 26836-07-7

Chemical Properties and Information

Synonyms: Dodecylbenzensulfonic acid,

ethanolamine salt

Molecular weight: 387.59
Melting Point: Not available
Water Solubility: Dispersible (E)
Vapor Pressure: <10⁻⁶ mm Hg (E)

Log₁₀ K_{ow}: Not available Log₁₀ K_{oc}: Not available Log₁₀ BCF: Not available Henry's Law: Not available

POTW Overall Removal Rate (%): 50-90 (E)

Chemistry of Use: Dispersant

C₂₀H₃₇NO₄S Structure:

$$\begin{bmatrix} \mathsf{CH}_3(\mathsf{CH}_2)_{1\,1} & & & \\ & & \mathsf{SO} \\ \mathsf{II} & & \\ \mathsf{O} & & & &$$

Boiling Point: Decomposes (E)

Density: 1 g/cm³ (E) Flash Point: Not available

Safety Hazard Factors: Not available

Benzenesulfonic Acid, Dodecyl-, Compounds with 2-**Propanamine**

CAS# 26264-05-1

Chemical Properties and Information

Synonyms: isopropylamine salt of

dodecylbenzenesulfonic

acid

Molecular weight: 385.5 Melting Point: Not available

Water Solubility: Dispersible (E) (surfactant)

Vapor Pressure: <10⁻⁵ mm Hg (E)

Log₁₀K_{ow}: Not available Log₁₀K_{oc}: Not available Log₁₀BCF: Not available Henry's Law: Not available

POTW Overall Removal Rate (%): 83-97 (E)

Chemistry of Use: Dispersant

 $C_{21}H_{39}NO_3S$ Structure:

Boiling Point: Decomposes (M)

Density: 1.03 g/cm³ (M) Flash Point: Not available

Safety Hazard Factors: Not available

Above data are either measured (M) or estimated (E)

Benzenesulfonic Acid, C₁₀-C₁₆-Alkyl Derivatives, Compounds with 2-Propanamine

CAS# 68584-24-7

Chemical Properties and Information

Synonyms: benzenesulfonic acid, C₁₀₋₁₆-alkyl

derivatives.

compounds with isopropylamine Molecular weight: 357-441

Melting Point: Not available

Water Solubility: Dispersible (surfactant) (E)

Vapor Pressure: <10⁻⁵ mm Hg (E)

Log₁₀K_{ow}: 4.78 (E) Log₁₀K_{oc}: 4.23 (E) Log₁₀BCF: 3.41 (E)

Henry's Law: 6.27X10⁻⁸ atm-m³/mole (E)

POTW Overall Removal Rate (%): 83-99 (E)

Chemistry of Use: Dispersant

 $C_{n+9}H_{2n+15}NSO_3$ (n=10-16) Structure:

Boiling Point: Decomposes (E)

Density: 1.05 g/cm³ (E) Flash Point: Not available

Safety Hazard Factors: Not available

Benzenesulfonic Acid, (Tetrapropenyl)-, Compound with 2-Propanamine

CAS# 157966-96-6

Chemical Properties and Information

Synonyms: Isopropylamine salt of (tetrapropenyl)

benzenesulfonic acid Molecular weight: 383.5 Melting Point: Not available

Water Solubility: Dispersible (E) (surfactant)

Vapor Pressure: <10⁻⁵ mm Hg (E)

 $Log_{10}K_{ow}$: Not available $Log_{10}K_{oc}$: Not available $Log_{10}BCF$: Not available Henry's Law: Not available

POTW Overall Removal Rate (%): 83-97 (E)

Chemistry of Use: Dispersant

C₂₁H₃₇NO₃S Structure:

 $\begin{bmatrix} \mathbf{R} - \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{I} & \mathbf{O} & \mathbf{I} \\ \mathbf{O} & \mathbf{O} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{O} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{O} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I}$

 $R = C_{12}H_{23}-$ branched, unsaturated

Boiling Point: Decomposes (E)

Density: 1.0 g/cm³ (E)
Flash Point: Not available

Safety Hazard Factors: Not available

Above data are either measured (M) or estimated (E)

Butyrolactone

CAS# 96-48-0

Chemical Properties and Information

Synonyms: γ-butyrolactone; dihydro-2(3H)-furanone; 1,2-butanolide; 1,4-butanolide; γ-hydroxybutyric acid lactone; 3-hydroxybutyric acid

lactone; 4-hydroxybutanoic acid lactone

Molecular weight: 86 Melting Point: -44°C (M) Water Solubility: miscible (M)

Vapor Pressure: 3.2 mm Hg (25° C)(M)

Log₁₀K_{ow}: -0.640 (M) Log₁₀K_{oc}: 0.85 (E) Log₁₀BCF: -0.72 (E)

Henry's Law: 1.81 x 10⁻⁵ atm-m³/mole (E) POTW Overall Removal Rate (%): 83-97 (E)

Chemistry of Use: Solvent

C₄H₆O₂ Structure:

0

Boiling Point: 204°C (M) Density: 1.125 g/mL (M)

Flash Point: Open cup: 98°C (M)

K_{oc}: 53 (E)

Physical state: Liquid Safety Hazard Factors:

Reactivity: 0 Flammability: 1 Ignitability: N

Cumene

CAS# 98-82-8

Chemical Properties and Information

Synonyms: benzene, (1-methylethyl)-;

Isopropylbenzene

Molecular weight: 120.19
Melting Point: -96°C (M)
Water Solubility: Insoluble (M)
Vapor Pressure: 3.53 mm Hg (M)

 $Log_{10}K_{ow}$: 3.66 (M) $Log_{10}K_{oc}$: 2.91 (E) $Log_{10}BCF$: 2.39 (E)

Henry's Law: 1.23X10⁻² atm-m³/mole (E) POTW Overall Removal Rate (%): 97-99 (E) Chemistry of Use: Solvent component Structure:

C₀H₁₂

CH(CH₃)₂

Boiling Point: 152-153°C (M) Density: 0.862 g/cm³ (M)

Flash Point: 39°C (closed cup) (M)

Safety Hazard Factors:

Reactivity: 1 Flammability: 3 Ignitability: Y

Above data are either measured (M) or estimated (E)

Diethanolamine

CAS# 111-42-2

Chemical Properties and Information

Synonyms: ethanol, 2,2'-iminobis-;

Iminodiethanol; 2,2'dihydroxyethylamine;
Molecular weight: 105.14
Melting Point: 28°C (M)
Water Solubility: Very soluble
Vapor Pressure: Not available

 $Log_{10}K_{ow}$: -1.43 (M) $Log_{10}K_{oc}$: -0.85 (E) $Log_{10}BCF$: -1.53 (E)

Henry's Law: <1.00X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 83.36-96.61

(E)

Chemistry of Use: Solvent

 $C_4H_{11}NO_2$

Structure: HOCH₂CH₂NHCH₂CH₂OH

Boiling Point: 270°C (M)
Density: 1.0881₄° g/mL (M)
Flash Point: 137°C (M)
Safety Hazard Factors:

Reactivity: 0 Flammability: 1 Ignitability: N

Diethylene Glycol Monobutyl Ether

CAS# 112-34-5

Chemical Properties and Information

Synonyms: 2-(2-butoxyethoxy) ethanol; butyl ethyl Cellosolve; diethylene glycol butyl ether; butyl Carbitol; Dowanol DB; Poly-Solv DB; butoxydiglycol, butyl digol, butyl diicinol

Molecular weight: 162.2 Melting Point: -68°C (M) Water Solubility: Miscible (E)

Vapor Pressure: 0.02 mm Hg (E) (20° C)

 $Log_{10}K_{ow}$: 0.56 (M) $Log_{10}K_{oc}$: -0.55 (E) $Log_{10}BCF$: 0.46 (E)

Henry's Law: <1.00X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 83-97 (E)

Chemistry of Use: Solvent

C₈H₁₈O₃

Structure: C₄H₉OCH₂CH₂OCH₂CH₂OH

Boiling Point: 231° C (M) Density: 0.954 g/mL (M)

Flash Point: Open cup: 110°C (M)

Closed cup: 78°C (M)

Safety Hazard Factors:

Reactivity: 0 Flammability: 1 Ignitability: N

Above data are either measured (M) or estimated (E)

Dimethyl Adipate

CAS# 627-93-0

Chemical Properties and Information

Synonyms: dimethyl hexanedioate; methyl

adipate; dimethyl ester adipic acid

Molecular weight: 174.25 Melting Point: 8°C (M)

Water Solubility: 0.1 g/L (E)

Vapor Pressure: 0.06 mm Hg (25°C)(E)

Log₁₀K_{ow}: 1.39 (E) Log₁₀K_{oc}: 1.04 (E) Log₁₀BCF: 0.82 (E)

Henry's Law: 1.28 x 10⁻⁷ atm-m³/mole (E) POTW Overall Removal Rate (%): 85-97 (E)

Chemistry of Use: Solvent

 $C_8H_{14}O_4$

Structure: (CH₃O)CO(CH₂)₄CO(OCH₃) Boiling Point: 193.7°C (at 760 mm Hg)(E)

Density: 1.063 g/mL (M) Flash Point: 107°C (M)

Physical state: Colorless, odorless liquid

Safety Hazard Factors:

Ignitability: N

Dimethyl Glutarate

CAS# 1119-40-0

Chemical Properties and Information

Synonyms: glutaric acid, dimethyl ester;

pentanedioic acid, dimethyl ester

Molecular weight: 160.17 Melting Point: -42.5°C (M) Water Solubility: 1 g/L (E) Vapor Pressure: 0.1 mm Hg (E)

 $Log_{10}K_{ow}$: 0.90 (E) $Log_{10}K_{oc}$: 0.77 (E) $Log_{10}BCF$: -0.14 (E)

Henry's Law: 9.09X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 97 (E)

Chemistry of Use: Solvent

C₇H₁₂O₄

Structure: CH₃O₂C(CH₂)₃CO₂CH₃

Boiling Point: 214°C (M) Density: 1.088 g/cm³ (M) Flash Point: 100°C (E) Safety Hazard Factors:

Ignitability: N

Above data are either measured (M) or estimated (E)

Dimethyl Succinate

CAS# 106-65-0

Chemical Properties and Information

Synonyms: succinic acid, dimethyl ester;

butanedioic acid,

dimethyl ester; methyl succinate

Molecular weight: 146.14 Melting Point: 19°C (M) Water Solubility: 8.3 g/L (M) Vapor Pressure: 0.1 mm Hg (E)

 $Log_{10}K_{ow}$: 0.19 (M) $Log_{10}K_{oc}$: 0.48 (E) $Log_{10}BCF$: Not available

Henry's Law: 5.8X10⁻⁶ atm-m³/mole (E) POTW Overall Removal Rate (%): 97 (E)

Chemistry of Use: Solvent

 $C_6H_{10}O_4$

Structure: CH₃O₂C(CH₂)₂CO₂CH₃

Boiling Point: 196.4°C (M) Density: 1.12 g/cm³ (M) Flash Point: 100°C (E) Safety Hazard Factors:

Ignitability: N

Dipropylene Glycol Monobutyl Ether

CAS# 29911-28-2

Chemical Properties and Information

Synonyms: 2-propanol, 1-(2-butoxy-1-

methylethoxy)-; DGMBE Molecular weight: 190.3 Melting Point: -73°C (M) Water Solubility: Miscible (E) Vapor Pressure: 0.044 mm Hg (M)

Log₁₀K_{ow}: 1.13 (E) Log₁₀K_{oc}: -0.15 (E) Log₁₀BCF: 0.63 (E)

Henry's Law: <1.00X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 83-97 (E)

Chemistry of Use: Solvent

C₁₀H₂₂O₃ Structure:

> H(OCHCH₂)₂OC₄H₉ | CH₃

Boiling Point: 229°C (M) Density: 0.913 g/cm³ (M)

Flash Point: 118° C (open cup) (M) Safety Hazard Factors: Not available

Above data are either measured (M) or estimated (E)

Dipropylene Glycol Methyl Ether

CAS# 34590-94-8

Chemical Properties and Information

Synonyms: glycol ether DPM; Dowanol DPM

Molecular weight: 148.2 Melting Point: -80°C (M) Water Solubility: Miscible (E)

Vapor Pressure: 0.4 mm Hg (M) (25°C)

 $Log_{10}K_{ow}$: -0.35 (E) $Log_{10}K_{oc}$: 1.00 (E) $Log_{10}BCF$: -0.49 (E)

Henry's Law: <1.00X10⁻⁸ atm-m³/mol (E) POTW Overall Removal Rate (%): 83-97 (E)

Chemistry of Use: Solvent

 $C_7H_{16}O_3$

Structure: CH₃CHOHCH₂OCH₂CH(OCH₃)CH₃

Boiling Point: 188.3°C (M) Density: 0.951 g/mL (M) Flash Point: 75°C (M) Physical state: Liquid Safety Hazard Factors:

Reactivity: 0 Flammability: 2 Ignitability: N

Distillates (Petroleum), Hydrotreated Middle

CAS# 64742-46-7

Chemical Properties and Information

Synonyms: hydrotreated middle distillate

Molecular weight: Varies Melting Point: -70°C (E) Water Solubility: 0.003 g/L (E) Vapor Pressure: 2 mm Hg (E)

 $Log_{10}K_{ow}$: 5.25 (E) $Log_{10}K_{oc}$: 3.24 (E) $Log_{10}BCF$: 3.76 (E)

Henry's Law: 5.3 atm-m³/mole (E)

POTW Overall Removal Rate (%): ≈ 100 (E)

Chemistry of Use: Solvent

 C_nH_{2n+2} and C_nH_{2n} (cycloparaffin)

Structure: No definite structure. Mixture of normal-, branched-, and cyclo-paraffins.

Boiling Point: 180-210°C (E) Density: 0.78 g/cm³ (E) Flash Point: 50°C (E) Safety Hazard Factors:

Ignitability: Y

Above data are either measured (M) or estimated (E)

Ethoxylated Nonylphenol

CAS# 9016-45-9, 26027-38-3, 68412-54-4

Chemical Properties and Information

Synonyms: poly(oxy-1,2-ethanediyl), α-

 $(nonylphenyl)-\Omega-hydroxy-;$ Antarox; polyethylene

glycol mono (nonylphenyl) ether

Molecular weight: 630 (for n=9.5) (typical range

500 - 800)

Melting Point: -20 to +10°C (E) Water Solubility: Soluble (M) Vapor Pressure: <10⁻⁶ mm Hg (E)

 $Log_{10}K_{ow}$: 3.93 (E) (np = 7) $Log_{10}K_{oc}$: -0.19 (E) (np = 7) $Log_{10}BCF$: Not available

Henry's Law: 1.81X10⁻²² atm-m³/mole (E)

(np = 7)

POTW Overall Removal Rate (%): 95 (M)^a Chemistry of Use: Nonionic surfactant $C_{34}H_{62}O_{10}$ (for n=9.5)

Structure:

Branched- C_9H_{19} $O(CH_2CH_2O)_nH$

n = 9.5 (for screen printing formulation product)

Boiling Point: >300°C (E) (decomposes)

Density: 0.8 g/cm³ (E) Flash Point: 200 - 260°C (E) Safety Hazard Factors:

Ignitability: N

^a Based on testing data (Weeks, J.A. et al. 1996. Proceedings of the CESIO 4th World Surfactants Congress, Barcelona, Spain. Brussels, Belgium: European Committee on Surfactants and Detergents, pp. 276-91.) the original estimate of POTW removal has been changed from 100% to 95% in the final report. This revision results in increased estimates of the releases from POTWs to surface waters as described in section 3.3. When the releases to surface water are compared with the concern concentration set at the default value of 0.001 mg/L, the formulations containing ethoxylated nonylphenols (formulations 4, 5, 7, 8, 9, 17, 24, and 40) present concerns to aquatic species that were not reported in the draft CTSA.

Ethylenediaminetetraacetic acid, tetrasodium salt

CAS# 64-02-8

Chemical Properties and Information

Synonyms: Glycine, N,N'-1,2-ethanediylbis[N-(carboxymethyl)-, tetrasodium salt; Tetrasodium

EDTA

Molecular weight: 380.20 Melting Point: >300°C (M) Water Solubility: 1030 g/L (M) Vapor Pressure: <10⁻⁷ mm Hg (E)

Log₁₀K_{ow}: Not available Log₁₀K_{oc}: Not available Log₁₀BCF: Not available Henry's Law: Not available

POTW Overall Removal Rate (%): 83.3-96.6 (E)

Chemistry of Use: Chelating agent

C₁₀H₁₂NaN₂O₈ Structure:

Na⁺ - OCCH₂ CH₂ CO Na⁺

Na⁺ - OCCH₂ NCH₂ CH₂ NCH₂ CO Na⁺

Na - OCCH₂ NCH₂ CH₂ NCH₂ CO Na⁺

O O

Boiling Point: Decomposes (E)

Density: 0.83 g/cm³ (E) Flash Point: Not available

Safety Hazard Factors: Not available

Above data are either measured (M) or estimated (E)

Fatty Acids, C₁₆-C₁₈, Methyl Esters

CAS# 67762-38-3

Chemical Properties and Information

Synonyms: fatty acid methyl esters

Molecular weight: 270-298
Melting Point: 27-36°C (M)
Water Solubility: <0.1 g/L (E)
Vapor Pressure: <10⁻³ mm Hg (E)

 $Log_{10}K_{ow}$: 7.74 (E) $Log_{10}K_{oc}$: 4.53 (E) $Log_{10}BCF$: 5.65 (E)

Henry's Law: 2.00X10⁻² atm-m³/mole (E) POTW Overall Removal Rate (%): 94-100 (E)

Chemistry of Use: Solvent

 $C_{n+2}H_{2n+4}O_2$ (n=15 to 17) and $C_{n+2}H_{2n+2}O_2$ (n=17)

Structure:

O || RCOCH₃

 $R = C_{15-17}$, and unsaturated C_{17}

Boiling Point: 325°C (E) Density: 0.88 g/cm³ (E) Flash Point: 200°C (E) Safety Hazard Factors:

Ignitability: N

Fatty Acids, C₁₆-C₁₈ and C₁₈-unsatd., Compounds with Diethanolamine

CAS# 68002-82-4

Chemical Properties and Information

Synonyms: diethanolamine tallate Molecular weight: 361-390 Melting Point: Not available Water Solubility: Dispersible (E) Vapor Pressure: <10⁻⁶ mm Hg (E)

 $Log_{10}K_{ow}$: 7.45 (E) $Log_{10}K_{oc}$: 3.80 (E) $Log_{10}BCF$: 5.43 (E)

Henry's Law: 5.23X10⁻⁵ atm-m³/mol (E) POTW Overall Removal Rate (%): 83-100 (E)

Chemistry of Use: Dispersant

 $C_{n+5}H_{2n+13}NO_4$ (n=15 to 17) and $C_{22}H_{45}NO_4$ Structure:

$$\begin{bmatrix} O \\ RCO \end{bmatrix} \begin{bmatrix} NH_2(CH_2CH_2OH)_2 \end{bmatrix}$$

$$R = C_{15-17}, \text{ and unsaturated } C_{17}$$

Boiling Point: Decomposes (E)

Density: >1 g/cm³ (E)
Flash Point: Not available

Safety Hazard Factors: Not available

Above data are either measured (M) or estimated (E)

Fatty acids, tall oil, Compounds with Diethanolamine

CAS# 61790-66-7

Chemical Properties and Information

Synonyms:

Molecular weight: 387 - 389
Melting Point: Not available
Water Solubility: Dispersible (E)
Vapor Pressure: <10⁻⁶ mm Hg (E)

Log₁₀K_{ow}: Not available Log₁₀K_{oc}: Not available Log₁₀BCF: Not available Henry's Law: Not available

POTW Overall Removal Rate (%): 83-100 (E)

Chemistry of Use: Dispersant

C₂₂H₄₅NO₄ and •C₂₂H₄₇NO₄ Structure:

$$\begin{bmatrix} O \\ R = c_{17} + c_{133} & \text{or } c_{17} + c_{135} \end{bmatrix}$$

$$R = c_{17} + c_{133} + c_{17} + c_{135}$$

Boiling Point: Decomposes (E)

Density: >1 g/cm³ (E) Flash Point: Not available

Safety Hazard Factors: Not available

Hydrocarbons, Terpene Processing By-Products

CAS# 68956-56-9

Chemical Properties and Information

Synonyms:

Molecular weight: ≥136
Melting Point: -40 to -60°C (E)
Water Solubility: 0.02 g/L (E)
Vapor Pressure: 1 mm Hg (E)

Log₁₀K_{ow}: 4.83 (E) Log₁₀K_{oc}: 3.12 (E) Log₁₀BCF: 3.44 (E)

Henry's Law: 3.80X10⁻¹ atm-m³/mole (E) POTW Overall Removal Rate (%): 98-100 (E)

Chemistry of Use: Solvent

C₁₀H₁₆ and larger

Structure: Mixture of C_{10} and larger terpenes.

Boiling Point: 165 - 180°C (E) Density: 0.84 - 0.87 g/cm³ (E) Flash Point: 30 - 50°C (E) Safety Hazard Factors:

Corrosivity: N

Above data are either measured (M) or estimated (E)

d-Limonene

CAS# 5989-27-5

Chemical Properties and Information

Synonyms: 1-methyl-4-(1-methylethenyl) cyclohexene: (+)-carvene: citrene: 1.8-*p*-

menthadiene; 4-isopropenyl-1-

methylcyclohexene cinene; cajeputene; kautschin

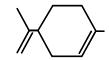
Molecular weight: 136
Melting Point: -74°C (M)
Water Solubility: 0.014 g/L (M)
Vapor Pressure: 5 mm Hg (E) (25°C)

Log₁₀K_{ow}: 4.83 (E) Log₁₀K_{oc}: 3.12 (E) Log₁₀BCF: 3.44 (E)

Henry's Law: 3.80X10⁻¹ atm-m³/mol (E) POTW Overall Removal Rate (%): >99 (E)

Chemistry of Use: Solvent

C₁₀H₁₆ Structure:



Boiling Point: 176°C (M) Density: 0.84 g/mL (M) Flash Point: 48°C (M) K_{oc}: 1,000 - 4,800 (E)

Safety Hazard Factors: Not available

Linalool

CAS# 78-70-6

Chemical Properties and Information

Synonyms: 1,6-octadien-3-ol, 3,7-dimethyl-

Molecular weight: 154.24 Melting Point: Not available

Water Solubility: Practically insoluble (M) Vapor Pressure: 0.29 mm Hg (M)

Log₁₀K_{ow}: 3.38 (E) Log₁₀K_{oc}: 1.75 (E) Log₁₀BCF: 2.34 (E)

Henry's Law: 4.23X10⁻⁵ atm-m³/mol (E) POTW Overall Removal Rate (%): 93-99 (E)

Chemistry of Use: Solvent

C₁₀H₁₈O Structure:



Boiling Point: 198-200°C (M) Density: 0.8622 g/cm³ (M) Flash Point: 74°C (E) Safety Hazard Factors:

Reactivity: 0 Flammability: 2 Ignitability: N

Above data are either measured (M) or estimated (E)

Mineral Spirits (Light Hydrotreated)

CAS# 64742-47-8

Chemical Properties and Information

Synonyms: many trade names by companies including Amsco, Apco, Epesol, Exxon, Phillips, Shell, etc., most of which include "mineral spirits"

in the name

Molecular weight: 86 for n-hexane; 112 for

ethycyclohexane, for example Melting Point: -60°C (E) Water Solubility: 0.001 g/L (E)

Vapor Pressure: 0.5-1 mm Hg (E) (25°C)

 $Log_{10}K_{ow}$: 3.90 (M) $Log_{10}K_{oc}$: 2.17 (E) $Log_{10}BCF$: 2.73 (E)

Henry's Law: 1.71 atm-m³/mole (E) POTW Overall Removal Rate (%): >99 (E)

Chemistry of Use: Solvent

Molecular formula: C_nH_{2n+2} (paraffin) and C_nH_{2n} (cycloparaffin)

Structure: Typical structures include normal paraffins,

CH₃(CH₂)_nCH₃, branched paraffins, and

cycloparaffins

Boiling Point: 140-180°C (M)
Density: 0.78 g/mL (M)
Flash Point: <43°C (M)
Physical State: Liquid
Safety Hazard Factors:

Reactivity: 0 Flammability: 2 Ignitability: Y

Naphtha (Petroleum), Hydrotreated Heavy

CAS# 64742-48-9

Chemical Properties and Information

Synonyms: aliphatic petroleum distillate C₉-C₁₁; naphthol spirits (aliphatic); hydrated lightstream cracked naphtha residuum (petroleum)

Molecular weight: 86 for n-hexane; 112 for

ethylcyclohexane, for example Melting Point: -80°C (E)

Water Solubility: 0.001 g/L (E)

Vapor Pressure: 1 mm Hg at 25°C (E)

 $Log_{10}K_{ow}$: 4.27 (E) $Log_{10}K_{oc}$: 2.70 (E) $Log_{10}BCF$: 3.01 (E)

Henry's Law: 3.01 atm-m³/mol (E)

POTW Overall Removal Rate (%): 99-100 (E)

Chemistry of Use: Solvent

C_nH_{2n+2} (paraffin) and C_nH_{2n} (cycloparaffin) Structure: No definite structure. Mixture of normal-, branched-, and cyclo-paraffins

Boiling Point: 66-230°C (M)
Density: 0.8 g/ml (E)
Flash Point: 60°C (M)
Safety Hazard Factors:

Reactivity: 0 Flammability: 4 Ignitability: Y Corrosivity: N

Above data are either measured (M) or estimated (E)

Nerol

CAS# 106-25-2

Chemical Properties and Information

Synonyms: 2,6-octadiene-1-ol, 3,7-dimethyl-,

Molecular weight: 154.24 Melting Point: <-15.4°C (M) Water Solubility: Insoluble (E) Vapor Pressure: 0.06 mm Hg (M)

 $Log_{10}K_{ow}$: 3.47 (E) $Log_{10}K_{oc}$: 1.85 (E) $Log_{10}BCF$: 2.41 (E)

Henry's Law: 5.89X10⁻⁵ atm-m³/mole (E) POTW Overall Removal Rate (%): 94-99 (E)

Chemistry of Use: Solvent

C₁₀H₁₈O Structure:

ОН

Boiling Point: 224-225°C (M) Density: 0.8756 g/cm³ (M) Flash Point: 77°C (M)

Safety Hazard Factors: Not available

N-Methylpyrrolidone

CAS# 872-50-4

Chemical Properties and Information

Synonyms: N-methylpyrrolidone [1-methyl-2-pyrrolidone; 1-methylazacyclopenta-2-one; N-

methyl-γ-butyrolactam]; NMP Molecular weight: 99.13 Melting Point: <-17 to -23°C (M)

Water Solubility: Miscible (M)

Vapor Pressure: 0.334 mm Hg (E) (25°C)

 $Log_{10}K_{ow}$: -0.38 (M) $Log_{10}K_{oc}$: 1.32 (E) $Log_{10}BCF$: -0.31 (E)

Henry's Law: 3.16X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 97 (E)

Chemistry of Use: Solvent

C₅H₉NO Structure:

⟨N CH.

Boiling Point: 202°C (M)

Density: 1.03 g/mL (M) Flash Point: 96°C (M) Safety Hazard Factors:

Reactivity: 1 Flammability: 3 Ignitability: Y

Above data are either measured (M) or estimated (E)

Oxirane, Methyl-, Polymer with Oxirane, Monodecyl Ether

CAS# 37251-67-5

Chemical Properties and Information

Synonyms: ethoxylated propoxylated decyl

alcohol

Molecular weight: Varies Melting Point: <-50°C (E)

Water Solubility: Dispersible (n=3 to 10) (E)

Miscible (n>10) (E)

Vapor Pressure: <10⁻⁴ mm Hg (E)

 $Log_{10}K_{ow}$: 3.26 (E) $Log_{10}K_{oc}$: 6.67 (E) $Log_{10}BCF$: 2.25 (E)

Henry's Law: <1.00X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 1-95 (E)

Chemistry of Use: Dispersant

Molecular formula varies

Structure:

 $c_{10}H_{21}(OCH_2CH)_m(OCH_2CH_2)_nOH$

Boiling Point: Decomposes (E)

Density: <1 g/cm³ (E)
Flash Point: Not available

Safety Hazard Factors: Not available

2-Pinanol

CAS# 473-54-1

Chemical Properties and Information

Synonyms: bicyclo[3.1.1]heptan-2-ol, 2,6,6-

trimethyl-

Molecular weight: 154.24 Melting Point: 60 - 80 °C (M) Water Solubility: <0.1 g/L (E) Vapor Pressure: 1.9x10⁻² mm Hg (E)

Log₁₀K_{ow}: 2.85 (E) Log₁₀K_{oc}: 1.73 (E) Log₁₀BCF: 1.94 (E)

Henry's Law: 1.90X10⁻⁶ atm-m³/mole (E) POTW Overall Removal Rate (%): 88-98 (E)

Chemistry of Use: Solvent

C₁₀H₁₈O Structure:

→ OH

Boiling Point: 220°C (M) Density: 1.01 g/cm³ (E) Flash Point: 65°C (E) Safety Hazard Factors:

Ignitability: N

Above data are either measured (M) or estimated (E)

Plinols

CAS# 72402-00-7

Chemical Properties and Information

Synonyms: cyclopentanol, 1,2-dimethyl-3-

(1-methylethenyl)-Molecular weight: 154.24 Melting Point: 93°C (M)

Water Solubility: Very slightly soluble (E) Vapor Pressure: <0.01 mm Hg (E)

 $Log_{10}K_{ow}$: 3.34 (E) $Log_{10}K_{oc}$: 1.74 (E) $Log_{10}BCF$: 2.31 (E)

Henry's Law: 1.34X10⁻⁵ atm-m³/mole (E) POTW Overall Removal Rate (%): 11-99 (E)

Chemistry of Use: Solvent

C₁₀H₁₈O Structure:

CH₃

Boiling Point: 220°C (E) Density: 0.92 g/cm³ (E) Flash Point: Not available

Safety Hazard Factors: Not available

Polyethoxylated Isodecyloxypropylamine

CAS# 68478-95-5

Chemical Properties and Information

Synonyms: poly(oxy-1,2-ethanediyl), α,α' -

(iminodi-2,1

ethanediyl) bis[ω -hydroxy]-, N-[3-(branched

decyloxy)propyl] derivatives Molecular weight: >400 Melting Point: Not available

Water Solubility: Dispersible or soluble (depending on degree of ethoxylation) (E)

Vapor Pressure: <10⁻⁶ mm Hg (E)

Log₁₀K_{ow}: 0.92 (E) Log₁₀K_{oc}: -1.43 (E) Log₁₀BCF: 0.47 (E)

Henry's Law: <1.00X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 85-97 (E)

Chemistry of Use: Dispersant

Molecular formula varies

Structure:

 $\begin{array}{c} \operatorname{Ho}(\operatorname{CH}_2\operatorname{CH}_2\operatorname{O})_{\operatorname{n}}\operatorname{CH}_2\operatorname{CH}_2\operatorname{NCH}_2\operatorname{CH}_2\operatorname{CH}_2(\operatorname{OCH}_2\operatorname{CH}_2)_{\operatorname{n}}\operatorname{OH} \\ | \\ \operatorname{CH}_2\operatorname{CH}_2\operatorname{CH}_2\operatorname{OR} \end{array}$

 $R = C_{10}H_{21} - branched$

Boiling Point: Decomposes (E)

Density: Not available
Flash Point: Not available

Safety Hazard Factors: Not available

Above data are either measured (M) or estimated (E)

Poly (Oxy-1,2-Ethanediyl), α -Hexyl- ω -Hydroxy-

CAS# 31726-34-8

Chemical Properties and Information

Synonyms: ethoxylated hexyl alcohol

Molecular weight: >278

Melting Point: -10°C (E)

Water Solubility: Dispersible (n=3 to 10),

Miscible (n>10) (E)

Vapor Pressure: <0.005 mm Hg (E)

Log₁₀K_{ow}: 0.73 (E) Log₁₀K_{oc}: 1.58 (E) Log₁₀BCF: 0.32 (E)

Henry's Law: <1.00X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 83-97 (E)

Chemistry of Use: Dispersant

 $C_{2n+6}H_{4n+14}O_{n+1}$ (n>3) Structure: $C_6H_{13}O(CH_2CH_2O)_nH$ (n>3) Boiling Point: >270°C (E)

Density: >0.95 g/cm³ (E)
Flash Point: >150°C (E)
Safety Hazard Factors:

Ignitability: N

Propanoic Acid, 3-Ethoxy-, Ethyl Ester

CAS# 763-69-9

Chemical Properties and Information

Synonyms: ethyl-3-ethoxy propionate; ethyl-β-

ethoxy propionate

Molecular weight: 146.1 Melting Point: -100°C (M)

Water Solubility: Slightly soluble (1 g/L) (E) Vapor Pressure: 0.9 mm Hg (at 20°C) (M)

 $Log_{10}K_{ow}$: 1.08 (E) $Log_{10}K_{oc}$: 0.61 (E) $Log_{10}BCF$: 0.59 (E)

Henry's Law: 4.77X10⁻⁷ atm-m³/mole (E) POTW Overall Removal Rate (%): 84-97 (E)

Chemistry of Use: Solvent

 $C_7H_{14}O_3$

Structure: CH₃CH₂OOCCH₂CH₂OCH₂CH₃

Boiling Point: 170°C (M) Density: 0.9496 g/cm³ (M)

Flash Point: 82°C (open cup) (M) Safety Hazard Factors: Not available

Above data are either measured (M) or estimated (E)

Propylene Glycol

CAS# 57-55-6

Chemical Properties and Information

Synonyms: 1,2-propanediol; methyl glycol; 1,2-

dihydroxypropane; methylethylene glycol;

trimethyl glycol

Molecular weight: 76.10 Melting Point: -60°C (M) Water Solubility: Miscible

Vapor Pressure: 0.2 mm Hg at 20°C (M)

Log₁₀K_{ow}: -0.92 (M) Log₁₀K_{oc}: 0.00 (E) Log₁₀BCF: -0.82 (E)

Henry's Law: 1.74x10⁻⁷atm-m³/mole (E) POTW Overall Removal Rate (%): 97 (E)

Chemistry of Use: Solvent

C₃H₈O₂

Structure: HOCH(CH₃)CH₂OH Boiling Point: 187.3 °C (M) Density: 1.038 g/mL (M) Flash Point: 101 °C (M) Safety Hazard Factors:

Reactivity: 0 Flammability: 1 Ignitability: N

Propylene Glycol Monobutyl Ether

CAS# 5131-66-8

Chemical Properties and Information

Synonyms: 2-propanol, 1-butoxy-

Molecular weight: 132 Melting Point: -100°C (M) Water Solubility: 64 g/L (M)

Vapor Pressure: <0.98 mm Hg at 20°C (M)

Log₁₀K_{ow}: 0.98 (E) Log₁₀K_{oc}: 0.11 (E) Log₁₀BCF: 0.52 (E)

Henry's Law: 4.88X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 83-97 (E)

Chemistry of Use: Solvent

 $C_7H_{16}O_2$

Structure: C₄H₉OCH₂CH(CH₃)OH

Boiling Point: 170°C (M) Density: 0.89 g/cm³ (E)

Flash Point: 59 (closed cup) (M)

Safety Hazard Factors:

Ignitability: Y

Above data are either measured (M) or estimated (E)

Sodium bis(Ethylhexyl) Sulfosuccinate

CAS# 577-11-7

Chemical Properties and Information

Synonyms: butanedioic acid, sulfo-, 1,4-bis(2-ethylhexyl) ester, sodium salt; sodium sulfosuccinate; Docusate sodium

Molecular weight: 444.37 Melting Point: Not available

Water Solubility: 15 g/L (at 25°C) (M) Vapor Pressure: <10⁻⁶ mm Hg (E)

 $Log_{10}K_{ow}$: 6.10 (E) $Log_{10}K_{oc}$: 5.02 (E) $Log_{10}BCF$: 4.40 (E)

Henry's Law: <1.00X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): nearly 100 (E)

Chemistry of Use: Surfactant

C₂₀H₃₇NaO₇S Structure:

Boiling Point: Not available
Density: Not available
Flash Point: Not available

Safety Hazard Factors: Not available

Sodium Hydroxide

CAS# 1310-73-2

Chemical Properties and Information

Synonyms: caustic soda; lye; sodium hydrate;

soda lye

Molecular weight: 39.9 Melting Point: 323°C (M) Water Solubility: 1,180 g/L (E)

Vapor Pressure: Negligible (E); 1 mm Hg (M)

(739°C)

Log₁₀K_{ow}: Not available

Log₁₀K_{oc}: Not available Log₁₀BCF: Not available Henry's Law: Not available

POTW Overall Removal Rate (%): Not available

Chemistry of Use: Caustic

NaOH

Structure: NaOH

Boiling Point: 1390°C (M)
Density: 2.13 g/mL (M)
Flash Point: Not applicable

Physical State: Deliquescent orthorhombic white

powder

Safety Hazard Factors:

Reactivity: 1 Flammability: 0 Ignitability: N Corrosivity: Y

Above data are either measured (M) or estimated (E)

Sodium Xylene Sulfonate

CAS# 1300-72-7

Chemical Properties and Information

Synonyms: benzenesulfonic acid, dimethyl-,

sodium salt

Molecular weight: 208.09 Melting Point: Not available Water Solubility: Very soluble (E) Vapor Pressure: <10⁻⁶ mm Hg (E)

Log₁₀K_{ow}: Not available Log₁₀K_{oc}: Not available Log₁₀BCF: Not available Henry's Law: Not available

POTW Overall Removal Rate (%): 83-97 (E)

Chemistry of Use: Hydrotrope

C₈H₉NaSO₃ Structure:

CH3 0 II SO-Na+

and other isomers

Boiling Point: Not available

Density: Not available

Flood Point: Not available

Flash Point: Not available

Safety Hazard Factors: Not available

Solvent Naphtha (Petroleum), Heavy Aromatic

CAS# 64742-94-5

Chemical Properties and Information

Synonyms: Aromatic 150; Comsolv 150 Molecular weight: 128 for naphthalene

Melting Point: -80°C (E)

Water Solubility: 0.03 g/L (M) for naphthalene Vapor Pressure: 0.5 mm Hg (E) (25°C)

Log₁₀K_{ow}: 4.45 (M) Log₁₀K_{oc}: 4.31 (E) Log₁₀BCF: 3.15 (E)

Henry's Law: 2.56X10⁻⁵ atm-m³/mole (E) POTW Overall Removal Rate (%): 96 (E)

Chemistry of Use: Solvent

C₁₀H₈ for naphthalene

Structure: Consist chiefly of aromatic hydrocarbons, including small fused-ring

compounds such as naphthalene

Boiling Point: 150-290°C (E) Density: 0.87 g/mL (E) Flash Point: 38°C (E) Physical State: Liquid Safety Hazard Factors:

Reactivity: 0 Flammability: 2 Ignitability: Y Corrosivity: N

Above data are either measured (M) or estimated (E)

Solvent Naphtha (Petroleum), Light Aliphatic

CAS# 64742-89-8

Chemical Properties and Information

Synonyms: VM&P #66; lacolene; rubber solvent; petroleum ether; naphtha; varnish makers' and

painters' solvent; VM&P Naphtha

Molecular weight: 86 for n-hexane: 112 for

ethycyclohexane, for example Melting Point: <-80°C (M) Water Solubility: 0.001 g/L (E) Vapor Pressure: 20 mm Hg (E) (25°C)

 $\begin{array}{l} Log_{10}K_{ow}\!\!: \; 3.44 \; (M) \\ Log_{10}K_{oc}\!\!: \; 2.22 \; (E) \\ Log_{10}BCF\!\!: \; 2.18 \; (E) \end{array}$

Henry's Law: 2.55X10⁻¹ atm-m³/mole (E) POTW Overall Removal Rate (%): >94 (E)

Chemistry of Use: Solvent

Molecular Formula: C_nH_{2n+2} (paraffin) and C_nH_{2n}

(cycloparaffin)

Structure: Typical structures include normal paraffins, CH₃(CH₂)₀CH₃, branched paraffins, and

cycloparaffins

Boiling Point: 35-160°C (M)
Density: 0.7 g/mL (E)
Flash Point: 0°C (E)
Physical State: Liquid
Safety Hazard Factors:

Reactivity: 0 Flammability: 3 Ignitability: Y Corrosivity: N

Solvent Naphtha (Petroleum), Light Aromatic

CAS# 64742-95-6

Chemical Properties and Information

Synonyms: Comsolv 100

Molecular weight: 128 for naphthalene

Melting Point: -80°C (E)

Water Solubility: 0.03 g/L (M) for naphthalene Vapor Pressure: 0.5 mm Hg (E) (25°C)

Log₁₀K_{ow}: 3.30 (M) Log₁₀K_{oc}: 3.26 (E)

Log₁₀BCF: 2.28 (E)

Henry's Law: 3.70X10⁻⁴ atm-m³/mole (E) POTW Overall Removal Rate (%): >92 (E)

Chemistry of Use: Solvent

C₁₀H₈ for naphthalene

Structure: Consist chiefly of aromatic hydrocarbons, including small fused-ring

compounds such as naphthalene Boiling Point: 135-210°C (E) Density: 0.87 g/mL (E)

Flash Point: 38°C (E)
Physical State: Liquid
Safety Hazard Factors:

Reactivity: 0 Flammability: 2 Ignitability: Y Corrosivity: N

Above data are either measured (M) or estimated (E)

Solvent Naphtha (Petroleum), Medium Aliphatic

CAS# 64742-88-7

Chemical Properties and Information

Synonyms: Solvent 140

Molecular weight: 86 for n-hexane; 112 for

ethycyclohexane, for example Melting Point: -60°C (M)

Water Solubility: 0.001 g/L (E) Vapor Pressure: 1 mm Hg at 25°C (E)

Log₁₀K_{ow}: 5.64 (M) Log₁₀K_{oc}: 3.77 (E) Log₁₀BCF: 4.51 (E)

Henry's Law: 9.35 atm-m³/mol (E)

POTW Overall Removal Rate (%): 99.98-100 (E)

Chemistry of Use: Solvent

C_nH_{2n+2} (paraffin) and C_nH_{2n} (cycloparaffin) Structure: No definite structure. Mixture of normal-, branched-, and cyclo-paraffins.

Boiling Point: 176-210°C (M) Density: 0.787 g/mL (M) Flash Point: 60°C (M) Safety Hazard Factors:

Reactivity: 0 Flammability: 2 Ignitability: Y Corrosivity: N

Sorbitan, Mono-9-Octadecenoate,

CAS# 1338-43-8

Chemical Properties and Information

Synonyms: sorbitan mono-oleate, (crillet 4)

Molecular weight: 428.44 Melting Point: <20°C (E) Water Solubility: Dispersible (M) Vapor Pressure: <10⁻⁶ mm Hg (E)

 $Log_{10}K_{ow}$: 5.89 (E) $Log_{10}K_{oc}$: 2.75 (E) $Log_{10}BCF$: 4.24 (E)

Henry's Law: <1.00X10⁻⁸ atm-m³/mol (E) POTW Overall Removal Rate (%): 99.98-100 (E)

Chemistry of Use: Dispersant

C₂₄H₄₄O₆ Structure:

HO CHOH

R = OC(CH₂)₇CH=CH(CH₂)₇CH₃

Boiling Point: Not available
Density: 1.0 g/cm³ (E)
Flash Point: Not available

Safety Hazard Factors: Not available

Above data are either measured (M) or estimated (E)

Sorbitan, Monododecanoate, Poly(Oxy-1,2-Ethanediyl) Derivatives

CAS# 9005-64-5

Chemical Properties and Information

Synonyms: polysorbate - 20; polyoxy ethylene (20) sorbitan monolaurate; Tween 20; Laurate of

polyoxyethylenic sorbitan Molecular weight: 1,180 Melting Point: Not available

Water Solubility: Completely soluble (M); 1000

g/L (E)

Vapor Pressure: <10⁻⁶ mm Hg (E)

Log₁₀K_{ow}: Not available Log₁₀K_{oc}: Not available Log₁₀BCF: Not available Henry's Law: Not available

POTW Overall Removal Rate (%): 83-97 (E)

Chemistry of Use: Dispersant

 $C_{54}H_{114}O_{26}\\ Structure:\\ \\ {}^{\text{Ho}(c_2H_4O)_{\text{w}}}\underbrace{-}_{0}\underbrace{-}_{\text{cH}(oc_2H_4)_{\text{y}}}\underbrace{-}_{0}H_{2}\underbrace{-}_{0}\underbrace{-}_{$

w+x+y+z = 20

Boiling Point: Not available Density: 1.1 g/cm³ (M)

Flash Point: 148°C (closed cup) (M)

Safety Hazard Factors:

Ignitability: N

Sorbitan, Monolaurate

CAS# 5959-89-7

Chemical Properties and Information

Synonyms: D-glucitol; 1,4-anhydro-, 6-

dodecanoate

Molecular weight: 358.34
Melting Point: <20°C (E)
Water Solubility: Insoluble (M)
Vapor Pressure: <10⁻⁶ mm Hg (E)

 $Log_{10}K_{ow}$: 3.15 (E) $Log_{10}K_{oc}$: 1.16 (E) $Log_{10}BCF$: 2.17 (E)

Henry's Law: <1.00X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 90-98 (E)

Chemistry of Use: Dispersant

C₁₈H₃₄O₆ Structure:

но он снон СН₂ осс 11 H₂₃

Boiling Point: 393°C (M)
Density: 1.0 g/cm³ (E)
Flash Point: Not available

Safety Hazard Factors: Not available

Above data are either measured (M) or estimated (E)

Sorbitan, Tri-9-Octadecenoate, Poly(Oxy-1,2-Ethanediyl) Derivatives

CAS# 9005-70-3

Chemical Properties and Information

Synonyms: sorbitan tri-oleate (crillet 45)

Molecular weight: 1,836 (n=20) Melting Point: Not available

Water Solubility: Completely soluble (E) Vapor Pressure: <10⁻⁶ mm Hg (E)

Log₁₀K_{ow}: Not available Log₁₀K_{oc}: Not available Log₁₀BCF: Not available Henry's Law: Not available

POTW Overall Removal Rate (%): 99.98-100 (E)

Chemistry of Use: Dispersant

C₁₀₀H₁₈₈O₂₈ (n=20) Structure:

 $R(C_2H_4O)_w$ $OC_2H_4)_xR$ $CH(OC_2H_4)_yOH$ $H_2C(OC_2H_4)_zR$

w+x+y+z = 20

 $\mathbf{R} = \underset{0}{\overset{\text{OC}(\mathsf{CH}_2)_7}{\mathsf{CH}} = \mathsf{CH}(\mathsf{CH}_2)_7 \mathsf{CH}_3}$

Boiling Point: Not available Density: 1.1 g/cm³ (E) Flash Point: 160°C (E) Safety Hazard Factors:

Ignitability: N

Soybean Oil, Methyl Ester

CAS# 67784-80-9

Chemical Properties and Information

Synonyms: soybean based methyl esters

Molecular weight: 295 Melting Point: -30°C (E) Water Solubility: Insoluble (E) Vapor Pressure: 0.01 mm Hg (E)

 $Log_{10}K_{ow}$: 7.80 (E) $Log_{10}K_{oc}$: 4.79 (E) Log₁₀BCF: 5.70 (E)

Henry's Law: 2.03X10⁻³ atm-m³/mol (E) POTW Overall Removal Rate (%): 94-100 (E)

Chemistry of Use: Solvent

 $C_{19}H_{36}O_{2}$ and $C_{19}H_{34}O_{2}$

Structure: RCOOCH₃ (R = $C_{17}H_{33}$ or $C_{17}H_{31}$)

Boiling Point: Decomposes (E) Density: 0.883 g/cm³ (E) Flash Point: 160-180°C (E)

Safety Hazard Factors:

Reactivity: 0 Flammability: 1 Ignitability: N

Above data are either measured (M) or estimated (E)

Soybean Oil, Polymerized, Oxidized

CAS# 68152-81-8

Chemical Properties and Information

Synonyms: oxidized soybean oil Molecular weight: Varies Melting Point: Not available Water Solubility: Insoluble (E) Vapor Pressure: <10⁻⁵ mm Hg (E)

 $Log_{10}K_{ow}$: 15.33 (E) $Log_{10}K_{oc}$: 13.73 (E) Log₁₀BCF: 11.42 (E)

Henry's Law: 1.00X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 99.98-100 (E)

Chemistry of Use:

Molecular formula varies Structure: No definite structure Boiling Point: Decomposes (E) Density: Not available Flash Point: Not available Safety Hazard Factors:

Reactivity: 0 Flammability: 1 Ignitability: N

Stoddard Solvent

CAS# 8052-41-3

Chemical Properties and Information

Synonyms: Rule 66 mineral spirits; quick-dry mineral spirits; 140 solvent; VM&P naphtha; dry

cleaners' solvent.

Molecular weight: 86 for n-hexane; 112 for

ethylcyclohexane, for example Melting Point: -70°C (M) Water Solubility: Insoluble (M)

Vapor Pressure: 1 mm Hg at 25°C (E)

 $Log_{10}K_{ow}$: 5.25 (E) $Log_{10}K_{oc}$: 3.24 (E) $Log_{10}BCF$: 3.58 (E)

Henry's Law: 5.3 atm-m3/mole (E)

POTW Overall Removal Rate (%): ≈ 100 (E)

Chemistry of Use: Solvent

C_nH_{2n+2} (paraffins), C_nH_{2n} (cycloparaffins) Structure: No definite structure. Mixture of normal-, branched-, and cyclo-paraffins

Boiling Point: 157-196°C (M)

Density: 0.787 (M)
Flash Point: 60°C (M)
Safety Hazard Factors:

Reactivity: 0 Flammability: 2 Ignitability: Y

Above data are either measured (M) or estimated (E)

Tall Oil, Special

CAS# 68937-81-5

Chemical Properties and Information

Synonyms: fatty acids, C₁₈ and C₁₈-unsatd., methyl esters, methyl stearate, methyl oleate

Molecular weight: 296-298

Melting Point: 36-39°C (E)

Water Solubility: Insoluble (M) (<0.1 g/L) (E)

Vapor Pressure: <10⁻³ mm Hg (E)

 $Log_{10}K_{ow}$: 7.74 (E) $Log_{10}K_{oc}$: 4.53 (E) $Log_{10}BCF$: 5.65 (E)

Henry's Law: 2.00X10⁻² atm-m³/mole (E)

POTW Overall Removal Rate (%): nearly 100 (E)

Chemistry of Use: Solvent

 $\mathrm{C_{19}H_{36}O_2}$ and $\mathrm{C_{19}H_{38}O_2}$

Structure: CH₃(CH₂)₁₆COOCH₃

and CH₃(CH₂)₇CH=CH(CH₂)₇COOCH₃

Boiling Point: 325°C (E) Density: 0.88 g/cm³ (E) Flash Point: 200°C (E) Safety Hazard Factors:

Ignitability: N

α-Terpineol

CAS# 98-55-5

Chemical Properties and Information

Synonyms: 3-cyclohexene-1-methanol, $\alpha,\alpha,4$ -

trimethyl-;

p-menth-1-en-8-ol Molecular weight: 154.24 Melting Point: 2°C (M)

Water Solubility: Slightly soluble (M) Vapor Pressure: 0.12 mm Hg (M)

 $Log_{10}K_{ow}$: 3.33 (E) $Log_{10}K_{oc}$: 1.76 (E) $Log_{10}BCF$: 2.30 (E)

Henry's Law: 3.15X10⁻⁶ atm-m³/mol (E) POTW Overall Removal Rate (%): 86-98 (E)

Chemistry of Use: Solvent

C₁₀H₁₈O Structure:

CH3 CH3

Boiling Point: 214-224°C (M) Density: 0.9338 g/cm³ (M) Flash Point: 90°C (M) Safety Hazard Factors:

Reactivity: 0 Flammability: 2 Ignitability: N

Above data are either measured (M) or estimated (E)

Terpinolene

CAS# 586-62-9

Chemical Properties and Information

Synonyms: cyclohexene, 1-methyl-4-(1-methylethylidene)-; p-mentha-1,4(8)-diene

Molecular weight: 136.16 Melting Point: Not available Water Solubility: Insoluble (M) Vapor Pressure: 0.49 mm Hg (M)

 $Log_{10}K_{ow}$: 4.88 (E) $Log_{10}K_{oc}$: 3.12 (E) $Log_{10}BCF$: 3.48 (E)

Henry's Law: 6.00X10⁻² atm-m³/mol (E)

POTW Overall Removal Rate (%): 90.06-99.95

(E)

Chemistry of Use: Solvent

C₁₀H₁₆ Structure:



Boiling Point: 183-185°C (M) Density: 0.864 g/cm³ (M)

Flash Point: 37.2°C (closed cup) (M)

Safety Hazard Factors:

Ignitability: Y Corrosivity: N

Tetrapotassium Pyrophosphate

CAS# 7320-34-5

Chemical Properties and Information

Synonyms: diphosphoric acid, tetrapotassium

salt; TKPP

Molecular weight: 330.34 Melting Point: 1090°C (M) Water Solubility: 1,870 g/L (M) Vapor Pressure: <10⁻⁶ mm Hg (E)

 $Log_{10}K_{ow}$: Not available $Log_{10}K_{oc}$: Not available $Log_{10}BCF$: Not available Henry's Law: Not available

POTW Overall Removal Rate (%): 0-25 (E)

Chemistry of Use: Sequestering agent

K₄O₇P₂ Structure:

Boiling Point: Decomposes (E)

Density: 2.33 g/cm³ (M)
Flash Point: Not available

Safety Hazard Factors: Not available

Above data are either measured (M) or estimated (E)

Xylene

CAS# 1330-20-7

Chemical Properties and Information

Synonyms: dimethylbenzene; methyltoluene;

xylol

Molecular weight: 106.2

Vapor Pressure: 10 mm Hg (E) (25°C)

Water Solubility: 0.1 g/L (E)
Melting Point: o: -25°C (M)

m: -48°C (M) p: 13°C (M)

Log₁₀K_{ow}: 3.15 (M) Log₁₀K_{oc}: -0.69 (E)

Log₁₀BCF: 2.16 (E)

Henry's Law: 1.81X10⁻⁸ atm-m³/mole (E) POTW Overall Removal Rate (%): 94 (E)

Chemistry of Use: Solvent

C₈H₁₀ Structure:

 CH_3 CH_3

Boiling Point: 137-140°C (M)

Density: 0.864 g/mL (M) Flash Point: o: 17°C (M)

m: 29°C (M) p: 27°C (M)

Physical State: Colorless liquid

Safety Hazard Factors:

Reactivity: 0 Flammability: 3 Ignitability: Y Corrosivity: N